Monte Carlo Simulation of Crystalline and Amorphous Polymeric Solid Nitrogen

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Non-molecular nitrogen solid in crystalline and amorphous phases is studied on the basis of a potential model proposed earlier for a cubic gauche polymeric crystal. The amorphous state was created by fast melting followed by instant quenching of crystalline structure. At certain conditions, the resulting amorphous solid was found to be stable enough to perform Monte Carlo simulation and to compute its thermodynamic and structural properties. At lower temperatures and higher densities, a negative thermal expansion was found in amorphous solid, as was formerly the case in the cubic gauche non-molecular nitrogen crystal. The shape of atom-atom distribution functions and analysis of crystalline vibrations reveal the particular characteristics of anharmonicity responsible for this effect.